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Efficient Gradient-Based Shape Optimization Using Viscous and Multiblock CFD Methodology

Oktay Baysal
Old Dominion University
Aerospace Engineering Department
Norfolk, VA 23529-0247

1.0 Summary of Progress

The first period of this three-year research project, supported by NASA Langley Research Center under NCC-1-211, was from March 9, 1995 to March 8, 1996. The major activity for this period has been the development of the *low-memory* methodology for the discrete-sensitivity-based shape optimization[1]. This was accomplished by solving all the resulting sets of equations using an alternating-direction-implicit (ADI) approach.

The formerly developed preconditioned-conjugate-gradient (PCG) solvers[2,3] for the analysis and the sensitivity equations had resulted in very large error reductions per iteration; quadratic convergence was achieved whenever the solution entered the domain of attraction to the root. Its memory requirement was also lower as compared to a direct inversion solver[4,5]. However, this memory requirement was high enough to preclude the realistic, high grid density design of a practical 3D geometry. This limitation served as the impetus to the first-year activity.

The results indicated that shape optimization problems which required large numbers of grid points could be resolved with a gradient-based approach. Therefore, to better utilize the computational resources, it was recommended that a number of coarse grid cases, using the PCG method, should initially be conducted to better define the optimization problem and the design space, and obtain an improved initial shape. Subsequently, a fine grid shape optimization should be conducted, using the ADI method, to accurately obtain the final optimized shape.

The minor activity during this period was the interaction with the members of the Aerodynamic and Aeroacoustic Methods Branch of Langley Research Center during one stage of their investigation to develop an adjoint-variable sensitivity method[6] using the viscous flow equations. This method had algorithmic similarities to the variational sensitivity[7] methods and the control-theory[8] approach. However, unlike the prior studies, it was considered for the three-dimensional, viscous flow equations.

2.0 Identification and Features of the Methodology

Based on the experiences gained thus far, certain recommendations can be made for the directions to be taken. Hence, the features of the present methodology are given in this section. Most are selected due to their virtues, however, some are recommended for the ease of their implementation.

2.1 Flowfield analysis

- governing equations: thin-layer Navier-Stokes equations[9,10] (primarily for systems with multiple components in close proximity), with a switch for the choice of dropping the diffusion terms and employing the Euler equations (for isolated configurations), in conservation form and generalized curvilinear coordinates
- CFD discretization: second-order accurate, upwind-biased (van Leer flux-vector split), cell-centered, finite volume discretization in space; either preconditioned conjugate-gradient for unfactored equations[2,3], or ADI[1] with pseudo-time (local time stepping) for factored equations
- van Albada limiter
- domain decomposition for structured grids using multiblock[11-13] (MB) concepts (contiguous lines normal to the interfaces)
- vector processing of data; parallel processing with the number of grid blocks assigned to each processor determined by a load-balancing strategy

2.2 Parameterization

- a general and easily differentiable surface parameterization[14] (in addition to surface grid points or shape-specific functions) for flexibility and to reduce the number of design variables; for the definition and redefinition of the surfaces to be shape optimized, employ Nth-degree Bezier-Bernstein polynomials
- use the same approach, but with lower-order polynomials, to curve-fit the various shape schedules[15]

2.3 Optimization algorithm

- gradient-based and constrained optimization algorithm, such as, the feasible-directions method[16]
- within the feasible region (no active constraints): deterministic search algorithms, such as, a univariate search strategy (sequential one-dimensional minimization in a multidimensional design space) with variable (using zeroth-order methods) alpha-step-size, or simply a constant-alpha-step-size (although less efficient for linear regions, better success rate for nonlinear regions)

- various options (user-changeable) of stopping criteria used for the optimization and for the flow analysis (either the convergence tolerances of different orders of magnitude, or the number of iterations, or both)
- for shape optimization, Bezier control points and other shape scales[1,15,17] (taper, thickness, twist, cant, etc.) the design variables (as opposed to the relative slopes at the surface grid points) to reduce their numbers
- allow for geometric as well as aerodynamic constraints

2.4 Sensitivities

- to obtain the sensitivity coefficients (gradients) implement both the direct and adjoint-variable methods[4,5] as one may be advantageous over the other depending on the problem in hand (number of design variables versus the number of aerodynamic constraints)
- consistent differentiation[18,19] of the CFD-discretized equations to obtain all the necessary terms in the sensitivity equation and the equations rendering the gradients
- writing the sensitivity equation for a multiblock grid with strong coupling of the sensitivities across the block interfaces; that is, employing the SADD[12] scheme
- a desirable capability is the representation of the Reynolds stresses by an algebraic model in the flow analysis equations; however, consistent differentiation of the currently available models (empirical with tunable parameters) for the sensitivities needs further studying; an approximate approach may be the automatic differentiation[20] of the turbulence modeling terms[20]

2.5 Solvers for algebraic systems

- to solve the large set of linear algebraic equations resulting from the sensitivity equation (or the adjoint-variable equations), have several inversion options in, both direct and iterative approaches as they all have their distinct niches depending on the problem in hand: naive Gauss elimination with banded storage[4,5], sparse-matrix method for symbolic factorization[4,5], a first-order iterative method (such as, solving the delta-form of the equations by an ADI method[1], also known as the incremental technique[19]), a conjugate-gradient-like method [such as, the restarting version of GMRES(`k,m`)][2,3] with several fill-in options for the preconditioners

2.6 Programming

- optimizer as the outer `do-loop`
- option for out-of-core storage
- judiciously segregating the case-dependent routines for ease of setting up for different problems

3.0 Utilization of Readily Available Methodologies for Present Objectives

In order to achieve the goals of the proposed investigation in a rather timely and cost-effective manner, whenever possible, the methodologies (and their computer codes) that may be readily available and, in some cases, may even be reasonably validated, should be utilized. This may be done in a number of ways ranging from a "black box" utilization to simply using as an illustrative example.

The following methodologies, given with their acronyms, may be put in this category: ADS,[16] ADOS,[17] AeSOP,[1,21] and ADIFOR.[20] It should be noted, however, although these methodologies may be somewhat general, some have their computer codes written for specific cases and they are intended to be "research codes."

ADOS: The three dimensional, aerodynamic shape optimization method, which include discrete "sensitivity analysis on decomposed computational domains" (SADD), was developed to handle complex configurations with multiple components. By virtue of the *substructuring* used for the large Jacobian matrix ($\partial R/\partial Q$), which results from the sensitivity equation for large size problems, this method utilizes relatively less computer memory than the single-grid approaches. It employs the general purpose, multiblock CFD code CFL3D,[11] to perform the flow analyses.

AeSOP: This "second generation" methodology is more efficient in computer time usage than ADOS, but, at this time, it is limited to single grids and solves only the Euler equations. Therefore, it can be used for less-complex geometries, less number of grid points, and no-interference cases. However, this code may also be used to shape optimize a component of a complex configuration with the other components and their grids excluded from the design domain but their "instantaneously frozen" effects included as boundary conditions. After a few design iterations, the entire domain may be updated with the analysis. Then, the optimization may be repeated for the single component with updated effects. This approach should yield "one-sided interference" during a given optimization iteration; however, with the user-in-loop for the analysis updates, mutual interference may be accounted for in somewhat a limited manner.

It should also be noted that AeSOP is currently being reinvestigated for possible reductions in computer memory utilization per grid point. Some of the iterative methods being tried seek ways of solving the sensitivity equation without having to form the Jacobian matrix on the left-hand side, but rather on the explicit right-hand side.[1]

ADS: This is somewhat a general purpose package of optimization methods with its genesis being for the structural mechanics. Nonetheless, it may be slightly modified to handle the aerodynamic problems. One of the main issues that often arise as a result of this switch in its application, is the limited suitability of its search strategies for the largely nonlinear design spaces encountered in solving the aerodynamic shape optimization problems. It has, however, all the capabilities desired in §2.3.

ADIFOR: In 1992, the author and his graduate students had unsuccessfully tried to use commercially available mathematical packages (MATHEMATICA™ and MACSYMA™), to perform the differentiation needed to obtain the sensitivities. Later that year, it was reported[20] that a mathematical tool, ADIFOR, was developed, and successfully demonstrated to obtain automatically the sensitivity coefficients from an existing CFD code. The output was also in the form of a computer code. One of the recent demonstrations used the code RAPID,[22,23] (interactive/batch version) which parameterized the geometry of a general aircraft configuration, generated its surface grid, and finally generated its grid sensitivities. Some recent research has also shown promise in eliminating the extra differential terms obtained in the process.

4.0 References

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